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On transition matrix elements between states in a Coulomb field. I

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With 2 figures in the text

Introduction

Calculation of transition matrix elements between states represented by Coulomb wave functions are important in many physical applications. Special cases of such matrix elements were considered by W. Gordon [1] and more recently K. Alder and A. Winther [2] have given general expressions and recursion formulas for the matrix elements, which are given in terms of hypergeometric functions of two variables. These functions are in many cases comparatively difficult to compute due to the lack of representations of the functions that lend themselves readily to computations Their series expansions often converge for limited values of the occurring parameters only and this restriction is sometimes a severe one. Integral representations often have the complexity of singular integrands unless detours of the path of integration are made into the complex plane. When relativistic effects are of importance, the non-integer steps of certain parameters decrease the usefulness of recursion relations and, as cross-sections may depend on a large number of matrix elements, it may be necessary to compute a considerable number of them directly.

In a previous paper by the present author [3] some aspects on Coulomb wave functions were given. The wave functions were expressed in terms of generalized hypergeometric functions in an attempt to increase the number of representations of the matrix elements as a result of the introduction of more general functions. As will be shown in this paper, the expressions obtained in [3] lead rather directly to simple expansions of certain matrix elements that are convergent for all values of the occurring parameters that have a physical meaning. The convergence of the expansions that will be presented is fastest for small energies. Standard treatment of the considered matrix elements leads to expansions that, for practical purposes, are best convergent for high energies.

Transition matrix elements between bound and non-bound states

Higher order perturbation calculations involve matrix elements between arbitrary Coulomb states or, more precisely, the calculation of matrix elements for transitions between non-bound states cannot be avoided. These matrix elements are sufficiently complicated to make such an undertaking as e.g. a rigorous calculation of Bremsstrahlung a very tedious matter even if a fast computor is used. The matrix elements entering into a first order pertubation calculation for transition from a bound to a non-bound state are simpler, particularly if the interaction may be written essentially as an exponential function as is the case when radiative interaction is caused by photons having well defined angular momentum. An example is internal conversion. In the similar process of external conversion or the photo effect, the incident photons must be described by a plane wave. The spherical symmetry of the problem necessitates expansion in multipoles if partial waves are to be used. The matrix elements entering into calculations of photo cross-sections are then of the same type as the matrix elements entering into calculations of internal conversion coefficients but they are more difficult to compute due to the fact that there is no predominant near-zone of the radiation field as is the case in internal conversion, where the radiation is emitted from the nucleus.

The following considerations will apply to matrix elements consisting essentially of integrals of the type:

$$I=\int_0^\infty e^{-\mu r}\, r^{q-1}\, e^{ikr}\, e^{-ipr}\, {}_1F_1\,(\gamma+i\eta;\,2\gamma;\,2ipr)\,dr. \tag{1}$$

Here $e^{-\mu r}$ and e^{ikr} may be thought of as the exponential functions entering into a bound wave function and a radiation field respectively. All parameters are intended to be real and positive. The function

$$e^{-ipr}\, {}_1F_1\,(\gamma+i\eta;\,2\gamma;\,2ipr) \tag{2}$$

is real valued and stands for a non-bound wave function, whereas r^q contains the occurring powers of r. Real expressions for the non-bound Coulomb wave functions, which are usually given as real and imaginary parts of a complex valued function, have been given in a previous paper [3]. The integral (1) is a special case of a more general integral computed by A. Erdélyi [4]. Termwise integration yields

$$\begin{aligned} I &= \int_0^\infty e^{-(\mu-ik+ip)r}\, r^{q-1}\, {}_1F_1\,(\gamma+i\eta;\,2\gamma;\,2ipr)\,dr= \\ &= \sum_{n=0}^{\infty}\frac{(\gamma+i\eta)_n\,(2ip)^n}{(2\gamma)_n\,n!}\int_0^\infty e^{-(\mu-ik+ip)r}\, r^{q+n-1}\,dr= \\ &= \sum_{n=0}^{\infty}\frac{(\gamma+i\eta)_n\,(2ip)^n}{(2\gamma)_n\,n!}\,\frac{\Gamma(q)\,(q)_n}{(\mu-ik+ip)^{q+n}}= \\ &= \frac{\Gamma(q)}{(\mu-ik+ip)^q}\,{}_2F_1\left(q,\,\gamma+i\eta;\,2\gamma;\,\frac{2ip}{\mu-ik+ip}\right). \end{aligned} \tag{3}$$

We have here used the power series expansions

$$ {}_1F_1(\gamma+i\eta;\,2\gamma;\,2ipr)=\sum_{n=0}^{\infty}\frac{(\gamma+i\eta)_n\,(2ipr)^n}{(2\gamma)_n\,n!} \tag{4}$$

$$ {}_2F_1\left(q,\,\gamma+i\eta;\,2\gamma;\,\frac{2ip}{\mu-ik+ip}\right)=\sum_{n=0}^{\infty}\frac{(q)_n\,(\gamma+i\eta)_n}{(2\gamma)_n\,n!}\left(\frac{2ip}{\mu-ik+ip}\right)^n \tag{5}$$

and the symbols

$$(\gamma+i\eta)_n=(\gamma+i\eta)\,(\gamma+1+i\eta)\,(\gamma+2+i\eta)\,\ldots\,(\gamma+n-1+i\eta)\quad \text{etc.}$$

$\Gamma(q)$ is the Γ-function of argument q. The series expansion (5) for the hypergeometric function in (3) converges when

$$\frac{2p}{|\mu-ik\pm ip|}<1. \tag{6}$$

The fact that the function (2) is real valued implies that

$$e^{-ipr}\,{}_1F_1(\gamma+i\eta;\,2\gamma;\,2ipr)=e^{ipr}\,{}_1F_1(\gamma-i\eta;\,2\gamma;\,-2ipr)$$

and thus the integral (1) does not change its value when the signs of p and η are changed simultaneously.

Then

$$I=\frac{\Gamma(q)}{(\mu-ik\pm ip)^q}\,{}_2F_1\left(q,\,\gamma\pm i\eta;\,2\gamma;\,\frac{\pm 2ip}{\mu-ik\pm ip}\right). \tag{7}$$

If the power series expansion is to be used for computing the matrix element, it is natural to choose the sign that makes the modulus of the argument smallest. Denoting the argument by z we have

$$z=-\frac{2ip}{\mu-i(k+p)}. \tag{8}$$

Let us investigate to some extent the possibilities of the expression (7) from a numerical point of view. A reasonably fast convergent power series expansion is beyond doubt the most convenient way of computing it except for special values of the parameters. It is convenient to have a special problem in mind and let us as an example choose internal conversion. Then the integral (7) is part of the expression for the probability that a bound electron is converted to a free electron with momentum p as a result of a nuclear transition. A competing process is the emission of γ-rays with wave number k. For conversion in the atomic K-shell we have $\mu=\alpha Z$, where α is the fine structure constant and Z is the nuclear charge number. The other parameters are

$$\gamma = \sqrt{1-\alpha^2 Z^2}$$

$$\eta = \frac{E \alpha Z}{p}$$

$$E = \sqrt{1+p^2}.$$

We are here considering relativistic wave functions. The parameter q depends on the nuclear spin change but will have no influence on the following arguments. Since γ-ray emission and conversion are competing processes following the same nuclear transitions we have

$$k = E - \gamma$$

expressing that the γ-ray energy is equal to the kinetic energy of the conversion electron plus its binding energy. Figure 1 shows the argument z as a function of k in the complex z-plane for $Z=82$. The trend of the curve is the same for all Z values.

The figures along the curve give the k-values in units of $mc^2 = 511$ kev. It is seen that the power series expansion (4) of (7) converges for $k < 0.3$ approximately where the curve cuts the unit circle. This corresponds to γ-ray energies less than 150 kev and conversion electron energies less than 50 kev approximately. For lower Z values, the k-values for which convergence ceases are smaller and most nuclear transitions of interest fall beyond the limit of convergence. Then analytic continuations of the ${}_2F_1$ function in terms of other ${}_2F_1$-functions can be used. E. M. Rose and collaborators used expansions in $1/z$ in their earlier calculations of internal conversion coefficients [5]. Figure 2 shows the reciprocal argument

$$z = \frac{\alpha Z - i(k-p)}{2ip}$$

as a function of k and the expansion is now seen to be convergent for $k > 0.25$ approximately.

The fact, that $z \to 1$ when $k \to \infty$ in figure 1, suggests expansion in powers of $1-z$ instead of $1/z$:

$$1 - z = 1 + \frac{2ip}{aZ - i(k+p)} = \frac{\alpha Z - i(k-p)}{\alpha Z - i(k+p)}.$$

It is easily seen that such an expansion is convergent for all k-values except possibly for the threshold value for conversion, which is the point 0 in fig. 1. We therefore use the well known analytic continuation of the hypergeometric function that changes the argument from z to $1-z$:

$$ {}_2F_1(a, b; c; z) = \frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)}\, {}_2F_1(a, b; a+b-c+1; 1-z) + $$

$$ + \frac{\Gamma(c)\,\Gamma(a+b-c)}{\Gamma(a)\,\Gamma(b)}\,(1-z)^{c-a-b}\, {}_2F_1(c-a, c-b; c-a-b+1; 1-z). $$

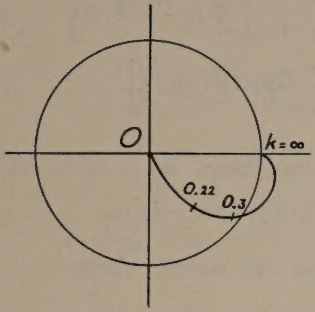

Fig. 1.

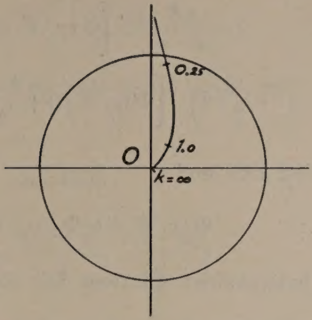

Fig. 2.

Then we obtain for the integral (7)

$$I=\frac{\Gamma(q)\,\Gamma(2\gamma)}{(\alpha Z-ik-ip)^{q}}\left\{\frac{\Gamma(\gamma-q+i\eta)}{\Gamma(2\gamma-q)\,\Gamma(\gamma+i\eta)}\cdot\right.$$

$$\cdot\,{}_2F_1\left(q,\,\gamma-i\eta;\,q-\gamma-i\eta+1;\,\frac{\alpha Z-ik+ip}{\alpha Z-ik-ip}\right)+$$

$$+\frac{\Gamma(q-\gamma-i\eta)}{\Gamma(q)\,\Gamma(\gamma-i\eta)}\left(\frac{\alpha Z-ik+ip}{\alpha Z-ik-ip}\right)^{\gamma-q+i\eta}\cdot$$

$$\left.\cdot\,{}_2F_1\left(2\gamma-q,\,\gamma+i\eta;\,\gamma-q+i\eta+1;\,\frac{\alpha Z-ik+ip}{\alpha Z-ik-ip}\right)\right\}. \tag{9}$$

The expression is relatively complicated considering the simplicity of the integral to be computed. The expansion in powers of $1/z$ leads to a very similar expression. It seems questionable whether these expressions are more practical to use than the calculation of the integral numerically without using analytical expressions.

In a previous paper, Coulomb wave functions were expressed with the aid of a confluent Appell function [3]. Calculations were carried out for the relativistic case. It was shown that the well known equations for the radial part of the Dirac equation:

$$\left.\begin{aligned}\frac{df}{dr}&=\frac{\varkappa-1}{r}\,f-\left(E-1+\frac{\alpha Z}{r}\right)g\\ \frac{dg}{dr}&=\left(E+1+\frac{\alpha Z}{r}\right)f-\frac{\varkappa+1}{r}\,g\end{aligned}\right\} \tag{10}$$

have solutions

$$\begin{aligned} f &= \frac{\alpha Z}{\varkappa-\gamma}\, t^{\gamma-1}\left[\Phi(\gamma,\, E,\, t) + \frac{E\varkappa+\gamma}{\varkappa+\gamma}\,\frac{t}{(2\gamma)_2}\,\Phi(\gamma+1,\, E,\, t)\right] \\ g &= t^{\gamma-1}\left[\Phi(\gamma,\, E,\, t) + \frac{E\varkappa+\gamma}{\varkappa-\gamma}\,\frac{t}{(2\gamma)_2}\,\Phi(\gamma+1,\, E,\, t)\right] \end{aligned} \tag{11}$$

where $t = 2\alpha Z r$ and

$$\Phi(\gamma,\, E,\, t) = \Phi_2(\gamma+i\eta,\, \gamma-i\eta;\, 2\gamma;\, ipr,\, -ipr). \tag{12}$$

Two independent solutions are obtained for two possible choices

$$\gamma = \pm\sqrt{\varkappa^2-\alpha^2 Z^2}.$$

The function $\Phi_2(\gamma+i\eta,\, \gamma-i\eta,\, 2\gamma,\, ipr,\, -ipr)$ is one of the confluent Appell functions which is defined as follows:

$$\Phi_2(b,\, b';\, c;\, x,\, y) = \sum_{\substack{m=0\\ n=0}}^{\infty} \frac{(b)_m (b')_n\, x^m y^n}{(c)_{m+n}\, m!\, n!}. \tag{13}$$

This series is convergent for all finite values of x and y. In [3] it was proved that the function (12) is reduced to more elementary functions when $b+b'=c$

$$\Phi_2(b,\, b';\, b+b';\, x,\, y) = e^y\, {}_1F_1(b,\, b+b';\, x-y). \tag{14}$$

This connects the solution (11) with more familiar expressions. The reduction (14) of the confluent Appell function seems to have first been given by Burchnall and Chaundy [6]. From (14), it follows easily that

$$e^{\lambda}\,\Phi_2(b,\, b';\, b+b';\, x,\, y) = \Phi_2(b,\, b';\, b+b';\, x+\lambda,\, y+\lambda), \tag{15}$$

valid for any λ. Thus an exponential function as factor results in the exponent being added to the argument of the function. From (11) it is clear that the integral (1) can now be written

$$I = \int_0^{\infty} e^{-(\mu-ik)r}\, r^{q-1}\,\Phi_2(\gamma+i\eta,\, \gamma-i\eta;\, 2\gamma;\, ipr,\, -ipr)\, dr \tag{16}$$

from which a simple expression for the integral may be derived. Using (15) we obtain

$$I = \int_0^{\infty} e^{-\mu r}\, r^{q-1}\,\Phi_2(\gamma+i\eta,\, \gamma-i\eta;\, 2\gamma;\, i(k+p)r,\, i(k-p)r)\, dr. \tag{17}$$

The expansion (13) is inserted and the resulting series is integrated term by term, which yields

$$I=\sum_{m,\,n}\frac{(\gamma+i\eta)_m\,(\gamma-i\eta)_n\,[i\,(p+k)]^m\,[i\,(k-p)]^n}{(2\,\gamma)_{m+n}\quad m!\;n!}\,\frac{\Gamma\,(q)\,(q)_{m+n}}{\mu^{q+m+n}}=$$

$$=\frac{\Gamma\,(q)}{\mu^q}\sum_{m,\,n}\frac{(q)_{m+n}\,(\gamma+i\eta)_m\,(\gamma-i\eta)_n}{(2\,\gamma)_{m+n}\,m!\;n!}\left(\frac{i\,(k+p)}{\mu}\right)^m\left(\frac{i\,(k-p)}{\mu}\right)^n.$$

This double series is the Appell function F_1 and thus

$$I=\frac{\Gamma\,(q)}{\mu^q}\,F_1\left(q,\,\gamma+i\eta,\,\gamma-i\eta;\,2\,\gamma;\,\frac{i\,(k+p)}{\mu},\,\frac{i\,(k-p)}{\mu}\right). \tag{18}$$

The series expansion of F_1 used above is convergent when the moduli of both arguments are less than unity [7], which means

$$\left|\frac{k\pm p}{\mu}\right|<1.$$

The function F_1 allows, however, a transformation

$$F_1\,(a,\,b,\,b';\,c;\,x,\,y)=(1-x)^{-b}\,(1-y)^{-b'}.\,F_1\left(c-a,\,b,\,b';\,c;\,\frac{x}{x-1},\,\frac{y}{y-1}\right), \tag{19}$$

and as the arguments in (18) are purely imaginary as a consequence of the use of the transformation (15), it is seen that the transformation (19) leads to an expression for the integral where the hypergeometric series defining F_1 is convergent for all values of the parameters that have a physical meaning. In addition, it is an expansion where the convergence is fastest for small energies. Using (19) we finally obtain

$$I=\frac{\Gamma\,(q)}{\mu^q}\left(\frac{\mu-i\,(k+p)}{\mu}\right)^{-\gamma-i\eta}\left(\frac{\mu-i\,(k-p)}{\mu}\right)^{-\gamma+i\eta}\cdot$$

$$\cdot F_1\left(2\,\gamma-q,\,\gamma+i\eta,\,\gamma-i\eta;\,2\,\gamma;\,\frac{i\,(k+p)}{i\,(k+p)-\mu},\,\frac{i\,(k-p)}{i\,(k-p)-\mu}\right). \tag{20}$$

There exist many expansions of F_1 in simple series but care must be taken not to loose the convergence when such an expansion is used. Among the possible expansions we select

$$F_1\,(a,\,b,\,b';\,c;\,x,\,y)=\sum_{n=0}^{\infty}\frac{(a)_n\,(b+b')_n}{(c)_n\quad n!}\,{}_2F_1\left(-n,\,b';\,b+b';\,1-\frac{y}{x}\right)x^n. \tag{21}$$

The derivation of (21) given by Appell and Kampé de Fériet [7] is based on the integral representation

$$F_1\,(a,\,b,\,b';\,c;\,x,\,y)=\text{const.}$$

$$\cdot\int_0^1\!\!\int_0^1 s^{b+b'-1}\,t^{b'-1}\,(1-s)^{c-b-b'-1}\,(1-t)^{b-1}\,[1-s\,(x+t\,y-t\,x]^{-a}\,d\,s\,d\,t \qquad (22)$$

where the last factor in the intergrand is expanded:

$$[1-s\,(x+t\,y-t\,x)]^{-a}=\sum_{n=0}^{\infty}\frac{(a)_n}{n!}\,s^n\,(x+t\,y-t\,x)^n. \qquad (23)$$

This expansion is inserted in (22). After term-wise integration, the expansion (21) is obtained. The expansion (23) is uniformly convergent when

$$|x+t\,y-t\,x|<1, \quad 0\leqslant t\leqslant 1. \qquad (24)$$

With the arguments of the function in (20) we have

$$x=\frac{i\,(k+p)}{i\,(k+p)-\mu}=\frac{(k+p)^2-i\,\mu\,(k+p)}{\mu^2+(k+p)^2}=\frac{1}{2}+\frac{1}{2}\,\frac{(k+p)^2-\mu^2-2\,i\,\mu\,(k+p)}{\mu^2+(k+p)^2}=$$

$$=\frac{1}{2}+\frac{1}{2}\,\frac{(k+p-i\,\mu)^2}{(k+p)^2+\mu^2}=\frac{1}{2}+\frac{1}{2}\,e^{i\varphi_1}$$

where
$$\varphi_1=2\ \text{arctg}\,\frac{\mu}{k+p}$$

because
$$\left|\frac{(k+p-i\,\mu)^2}{(k+p)^2+\mu^2}\right|=1\,.$$

Similarly
$$y=\frac{1}{2}+\frac{1}{2}\,e^{i\varphi_2},\quad \varphi_2=2\ \text{arctg}\,\frac{\mu}{k-p}\cdot$$

The two points x and y are thus always found on a circle in the complex plane with radius $1/2$ and its center at the point $1/2$. No points on the periphery of this circle are situated outside the unit circle and the point $x+t\,y-t\,x$ is never outside the smaller circle with radius $1/2$ as it is always found on a straight line having x and y as end points. This proves the convergence of the expansion (21).

The expansion of our expression (18) is then finally

$$I=\frac{\Gamma\,(q)}{\mu^q}\left[\frac{\mu-i\,(k+p)}{\mu}\right]^{-\gamma-i\eta}\left[\frac{\mu-i\,(k-p)}{\mu}\right]^{-\gamma+i\eta}\cdot$$

$$\cdot\sum_{n=0}^{\infty}\frac{(2\,\gamma-q)_n}{n!}\;{}_2F_1\left(-n,\,\gamma-i\,\eta;\,2\,\gamma;\,1-\frac{y}{x}\right)x^n=$$

$$=\frac{\Gamma\,(q)}{\mu^q}\left[\frac{\mu-i\,(k+p)}{\mu}\right]^{-\gamma-i\eta}\left[\frac{\mu-i\,(k-p)}{\mu}\right]^{-\gamma+i\eta}\sum_{n=0}^{\infty}c_n\,. \qquad (25)$$

For practical purposes, the terms c_n are most conveniently calculated from the recursion formula

$$c_{n+1} = \frac{2\gamma - q + n}{(2\gamma + n)(n+1)} \{[(n+\gamma)(x+y) + i\eta(x-y)]\, c_n - (2\gamma - q + n - 1)\, x y\, c_{n-1}\} \quad (26)$$

which is obtained from the recursion formulas for the hypergeometric functions.

The expression (25) may serve as an example of a useful result that follows rather directly using the new representation of the Coulomb wave functions (11). It is not claimed that expansions as simple as (25) cannot be derived starting from standard expressions for the wave functions but in so doing it seems to be accomplished in a much less direct way. An attractive feature is the occurrence of only the sum and difference of the linear momenta of the photons and electrons in the arguments and perhaps this symmetry will be helpful in studying more general matrix elements than the simple ones studied above.

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